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# UNDERSTANDING TWINNING NUCLEATION AND DISLOCATION CORE STRUCTURE THROUGH INTERSCALE HYBRID METHOD

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## ABSTRACT

The variety of emerging simulation methods and improved computational power advance the understanding in nanometals as a good compensation of the experiments. In this paper, the first principle methods are discussed, especially as a useful combination of the classical molecular dynamics, to overcome the disadvantages of the latter method. Two examples are given as: the nucleation of the {10-12} deformation twinning in magnesium, and the screw dislocation core structure with/without hydrogen in tungsten.

## 1. INTRODUCTION

The growing field of computational science witnesses the emerging numerical techniques for the solution of mathematical equations arising in all areas of physics. Improved algorithm and increased computational power broaden the application of different computational methods, allowing unprecedented access to the investigation of electrical and mechanical properties where experiments are difficult to perform or the detailed processes or mechanisms are difficult to reveal through experiments. This variety of state-of-the-art theoretical and computational methods in electronic structure theory and classical molecular dynamics has been developed to interpret the specific physical and mechanical problems in materials science and solid-state physics. However, there are bottlenecks between different methods and approximations pay a price on the accuracy of the results. So, the awareness of the bottlenecks of these methods in the nanometer scale is important to materials scientists majoring in the nano-metals. On this base, the definition of a subject, and the selection of methods and/or potentials can be optimized to reduce the cost and time. In this paper, the merits and bottlenecks of molecular dynamics and first principle calculation based on density functional theory (DFT) are summarized and two cases are given to demonstrate the principle mentioned above.

produced the same splitting core structures as expected, while Zhou's potential is different. This discrepancy, again, emphasizes the importance of the verification of potentials in advance of a serious calculation of different dislocation core structure.

In Fig. 5, hydrogen atoms are introduced in the tetrahedral position between tungsten atoms. The system we studied here is limited to one complex-layer of atoms in a  $\langle 111 \rangle$  direction which is composed of three layers of  $\{111\}$  atoms indexed by different colors and A, B and C. The whole system is periodic in the  $z$  ( $\langle 111 \rangle$ ) direction, thus the hydrogen concentration is about 0.22/nm. The initial position of the hydrogen atoms are in the octagonal position, after the relaxation they moves to the tetragonal position of the bcc crystal frames. Consequently, the core structures are obviously different compared to the hydrogen-free system. The splitting is not happening in three  $\{112\}$  planes any more, but with an expansion in the  $[001]$  direction. More ongoing detailed investigations focus on the different behaviors of dislocation core interactions and the mobility of a dislocation core in the presence of hydrogen atoms.

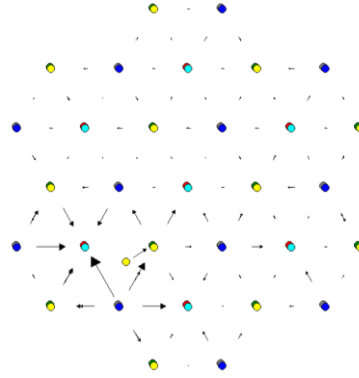


Fig. 5. Screw dislocation core structure with a hydrogen atom.

#### 4. CONCLUSIONS

In this short paper, the application of DFT and MD calculations in the studies of nano scale metallic deformation mechanism were discussed, especially in the cases of the gamma surface of Mg and the dislocation core structure of W. DFT and MD calculations can be a good compensation to each other, and more emphasis is laid on DFT calculations in this paper. With the help of DFT, a modified MD calculation can be more accurate, and at the same time more detailed information can be obtained from these hybrid methods. By doing this, the shortcomings of a MD calculation can be overcome, such as the mismatch between different potentials, and the inability to deal with a system with multi-elements. Combined with large scale parallel calculation, this method will show its great potential with diverse and universal applications especially in the multi-components systems.

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